

Procedure for Modeling Complexes

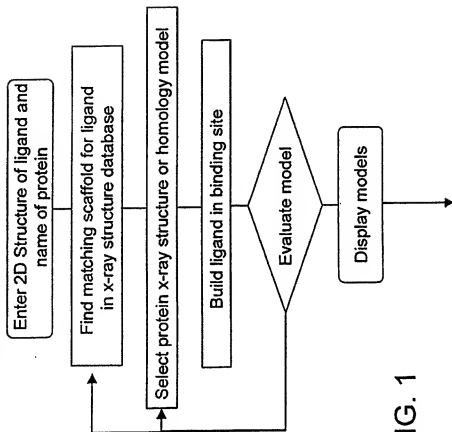
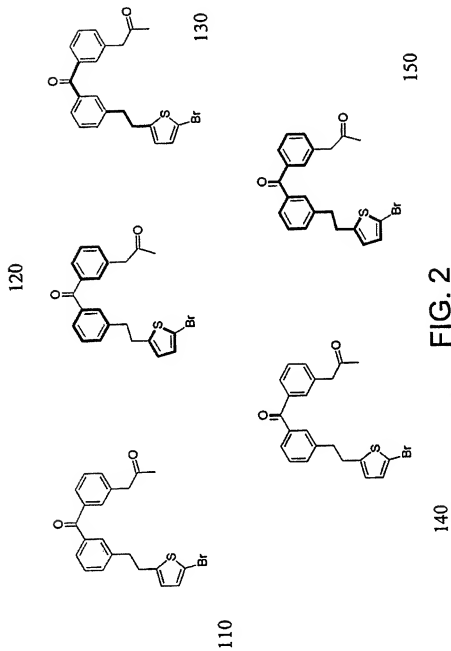


FIG. 1



Maximum Common Substructure

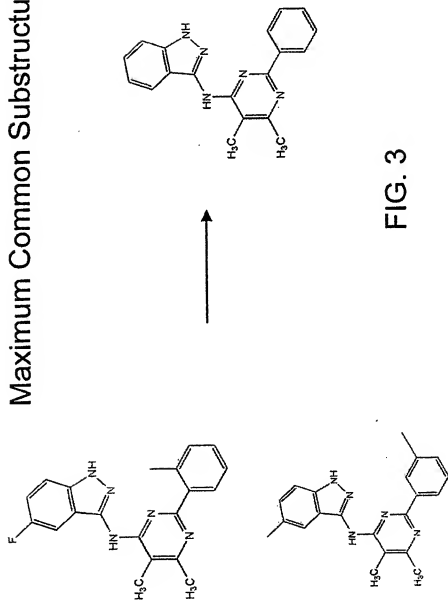


FIG. 3

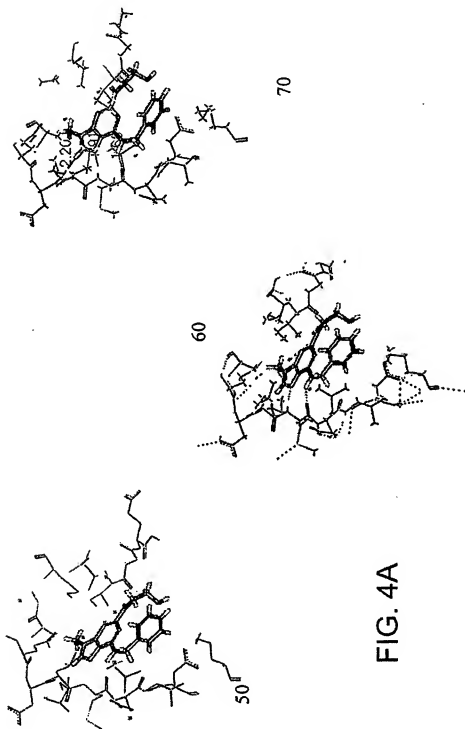
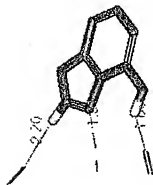
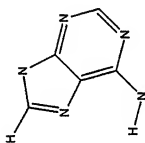


FIG. 4A

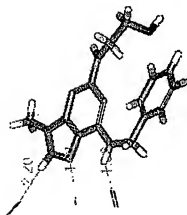


90

FIG. 4B



100



80

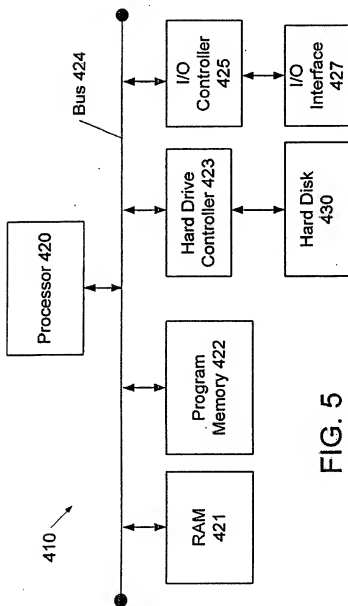


FIG. 5

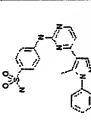
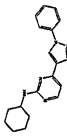
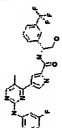
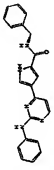
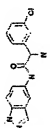
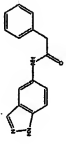
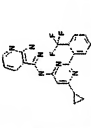
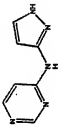
query ligand	protein	scaffold	rmsd (model vs. x-ray) / Angstrom
	ink3		0.9 - 1.3
	erk2		1.5 - 2.0
	pka (5xm)		1.2
	gsk3β		1.3 - 2.2

FIG. 6

FIG. 7A

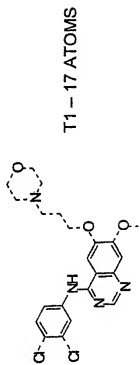


FIG. 7B

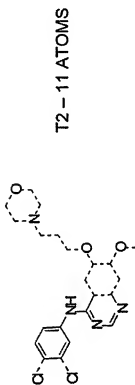
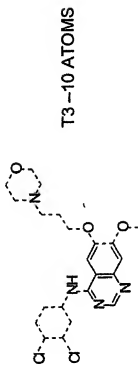


FIG. 7C



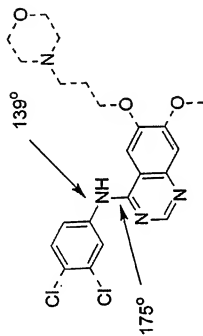


FIG. 8

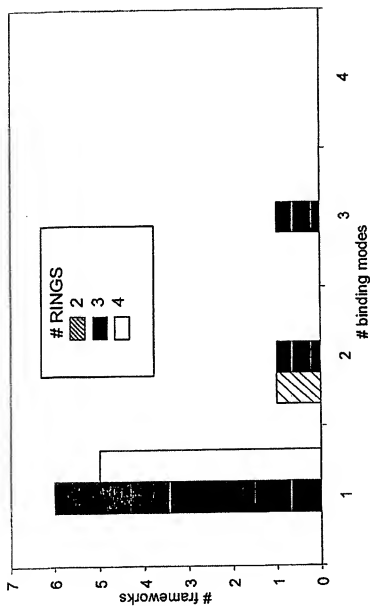


FIG. 9

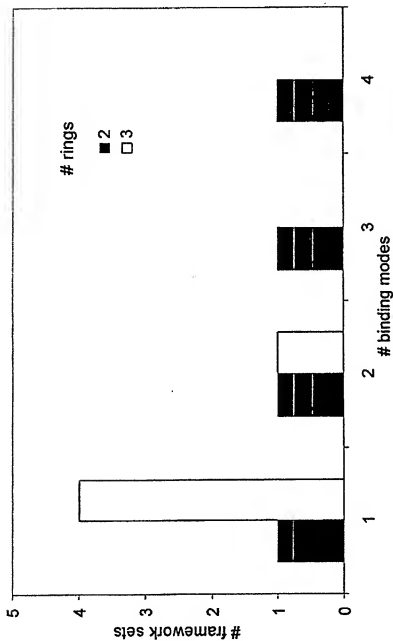


FIG. 10

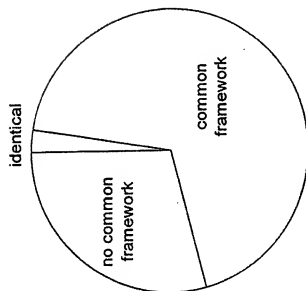


FIG. 11

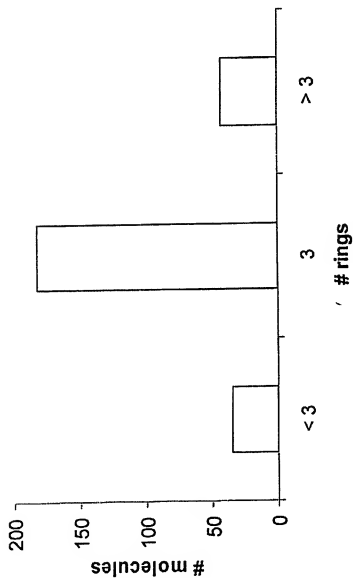
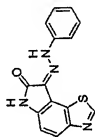
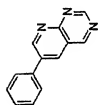


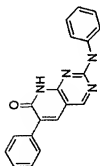
FIG. 12



10



9



8

FIG. 13